

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041724\
 Data File : VX041134.D
 Acq On : 17 Apr 2024 18:48
 Operator : JC/MD
 Sample : P2039-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E1CY1

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M

Title : VOC Analysis

Signal : TIC: VX041134.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	34	rBV2	3107	3048	0.29%	0.037%
2	1.368	43	46	59	rBV	93327	145054	13.68%	1.781%
3	1.648	88	92	109	rVB	50843	99032	9.34%	1.216%
4	2.288	191	197	210	rVB	216506	346869	32.71%	4.258%
5	2.782	273	278	289	rBV	5468	12317	1.16%	0.151%
6	3.123	333	334	338	rVB2	135	166	0.02%	0.002%
7	3.160	338	340	342	rBV	119	143	0.01%	0.002%
8	3.337	367	369	370	rBV	161	145	0.01%	0.002%
9	3.440	381	386	387	rBV	307	336	0.03%	0.004%
10	3.544	400	403	404	rBV2	180	188	0.02%	0.002%
11	3.593	404	411	417	rVV4	603	1483	0.14%	0.018%
12	3.776	440	441	444	rBV	161	148	0.01%	0.002%
13	3.831	448	450	453	rVV2	145	136	0.01%	0.002%
14	3.910	461	463	466	rVB2	143	134	0.01%	0.002%
15	4.062	483	488	489	rBV2	195	228	0.02%	0.003%
16	4.221	512	514	516	rBV2	149	150	0.01%	0.002%
17	4.239	516	517	521	rVB2	211	167	0.02%	0.002%
18	4.269	521	522	526	rBV2	169	143	0.01%	0.002%
19	4.367	536	538	541	rBV2	149	154	0.01%	0.002%
20	4.471	546	555	578	rBV	61779	227615	21.47%	2.794%
21	4.879	621	622	626	rVB2	226	204	0.02%	0.003%
22	4.922	626	629	630	rVB2	165	156	0.01%	0.002%
23	5.056	638	651	668	rBV	134553	413680	39.02%	5.078%
24	5.202	673	675	676	rBV2	350	265	0.02%	0.003%
25	5.306	690	692	694	rVB	290	205	0.02%	0.003%
26	5.385	699	705	706	rBV2	546	823	0.08%	0.010%
27	5.556	727	733	735	rBV2	670	1357	0.13%	0.017%
28	5.702	754	757	760	rVB2	175	195	0.02%	0.002%
29	5.842	778	780	781	rBV	192	141	0.01%	0.002%
30	5.964	788	800	819	rBV2	364966	1060293	100.00%	13.015%
31	6.348	855	863	874	rBV3	5365	16720	1.58%	0.205%
32	6.543	893	895	898	rBV2	203	244	0.02%	0.003%
33	6.672	912	916	918	rBV3	116	172	0.02%	0.002%
34	6.757	921	930	947	rBV	257408	629028	59.33%	7.721%
35	7.117	983	989	996	rVB4	1775	4308	0.41%	0.053%
36	7.214	999	1005	1012	rBV5	1285	2795	0.26%	0.034%

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Integrator: RTE

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M
 Title : VOC Analysis

37	7.306	1012	1020	1036	rBV	211083	465436	43.90%	5.713%
38	7.488	1046	1050	1055	rVB4	866	966	0.09%	0.012%
39	7.659	1073	1078	1085	rBV2	2852	7584	0.72%	0.093%
40	7.805	1096	1102	1115	rBV	51244	101485	9.57%	1.246%
41	8.153	1157	1159	1161	rVB	178	132	0.01%	0.002%
42	8.324	1181	1187	1203	rBV	125574	212380	20.03%	2.607%
43	8.555	1217	1225	1234	rBV	17316	32008	3.02%	0.393%
44	8.647	1234	1240	1255	rBV	513440	827485	78.04%	10.157%
45	8.952	1284	1290	1306	rBV2	96771	158717	14.97%	1.948%
46	9.202	1329	1331	1333	rBV	125	131	0.01%	0.002%
47	9.250	1333	1339	1347	rBV	24616	39627	3.74%	0.486%
48	9.317	1347	1350	1351	rBV2	1665	1676	0.16%	0.021%
49	9.391	1357	1362	1373	rBV	306513	492699	46.47%	6.048%
50	9.488	1374	1378	1390	rVB	36203	57077	5.38%	0.701%
51	9.586	1390	1394	1404	rVB	11624	19589	1.85%	0.240%
52	9.787	1426	1427	1430	rBV	195	223	0.02%	0.003%
53	9.848	1434	1437	1438	rBV	181	137	0.01%	0.002%
54	9.915	1443	1448	1465	rBV	72962	105616	9.96%	1.296%
55	10.055	1465	1471	1491	rVV	512983	725494	68.42%	8.905%
56	10.305	1506	1512	1517	rBV4	1006	2149	0.20%	0.026%
57	10.378	1521	1524	1527	rVB2	184	265	0.02%	0.003%
58	10.427	1527	1532	1533	rVB2	168	243	0.02%	0.003%
59	10.457	1533	1537	1538	rBV	177	134	0.01%	0.002%
60	10.488	1538	1542	1544	rBV	173	192	0.02%	0.002%
61	10.524	1544	1548	1550	rBV4	671	1012	0.10%	0.012%
62	10.646	1564	1568	1579	rVB2	3323	5922	0.56%	0.073%
63	10.732	1579	1582	1583	rBV2	161	134	0.01%	0.002%
64	10.835	1596	1599	1603	rBV2	166	330	0.03%	0.004%
65	10.890	1607	1608	1610	rVV2	227	129	0.01%	0.002%
66	10.957	1617	1619	1624	rVB2	250	327	0.03%	0.004%
67	11.000	1624	1626	1629	rBV	157	143	0.01%	0.002%
68	11.098	1639	1642	1647	rBV3	416	569	0.05%	0.007%
69	11.189	1652	1657	1670	rVV	402726	534146	50.38%	6.557%
70	11.317	1675	1678	1682	rVV2	766	1018	0.10%	0.012%
71	11.360	1682	1685	1687	rVV	263	196	0.02%	0.002%
72	11.457	1699	1701	1704	rVB2	226	239	0.02%	0.003%
73	11.488	1704	1706	1709	rVB2	163	162	0.02%	0.002%
74	11.567	1716	1719	1720	rBV2	170	178	0.02%	0.002%
75	11.707	1740	1742	1744	rBV	181	142	0.01%	0.002%
76	11.750	1747	1749	1750	rBV	297	213	0.02%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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 Title : VOC Analysis

77	11.969	1783	1785	1786	rBV	365	361	0.03%	0.004%
78	12.024	1789	1794	1805	rVV	494023	643347	60.68%	7.897%
79	12.274	1833	1835	1837	rBV	256	194	0.02%	0.002%
80	12.317	1837	1842	1861	rVV	556777	732045	69.04%	8.986%
81	12.622	1889	1892	1897	rBV	239	433	0.04%	0.005%
82	12.683	1899	1902	1903	rBV2	144	156	0.01%	0.002%
83	12.762	1911	1915	1919	rVB2	679	1021	0.10%	0.013%
84	12.811	1922	1923	1928	rVB2	194	187	0.02%	0.002%
85	12.859	1928	1931	1933	rBV2	127	140	0.01%	0.002%
86	12.908	1937	1939	1941	rBV2	159	143	0.01%	0.002%
87	13.122	1971	1974	1977	rVB2	300	339	0.03%	0.004%
88	13.183	1982	1984	1987	rVB2	120	165	0.02%	0.002%
89	13.213	1987	1989	1993	rBV	118	169	0.02%	0.002%
90	13.451	2024	2028	2030	rBV	138	171	0.02%	0.002%
91	13.591	2049	2051	2052	rVV2	337	276	0.03%	0.003%
92	13.621	2055	2056	2058	rBV	195	171	0.02%	0.002%
93	13.707	2066	2070	2071	rBV3	192	163	0.02%	0.002%
94	13.786	2081	2083	2086	rBV2	244	341	0.03%	0.004%
95	13.884	2097	2099	2100	rBV2	218	194	0.02%	0.002%
96	14.127	2136	2139	2143	rVB2	1118	1207	0.11%	0.015%
97	14.390	2181	2182	2187	rVB2	249	212	0.02%	0.003%
98	14.426	2187	2188	2190	rBV2	232	180	0.02%	0.002%
99	14.469	2194	2195	2197	rBV2	270	230	0.02%	0.003%
100	15.200	2313	2315	2317	rBV2	466	386	0.04%	0.005%

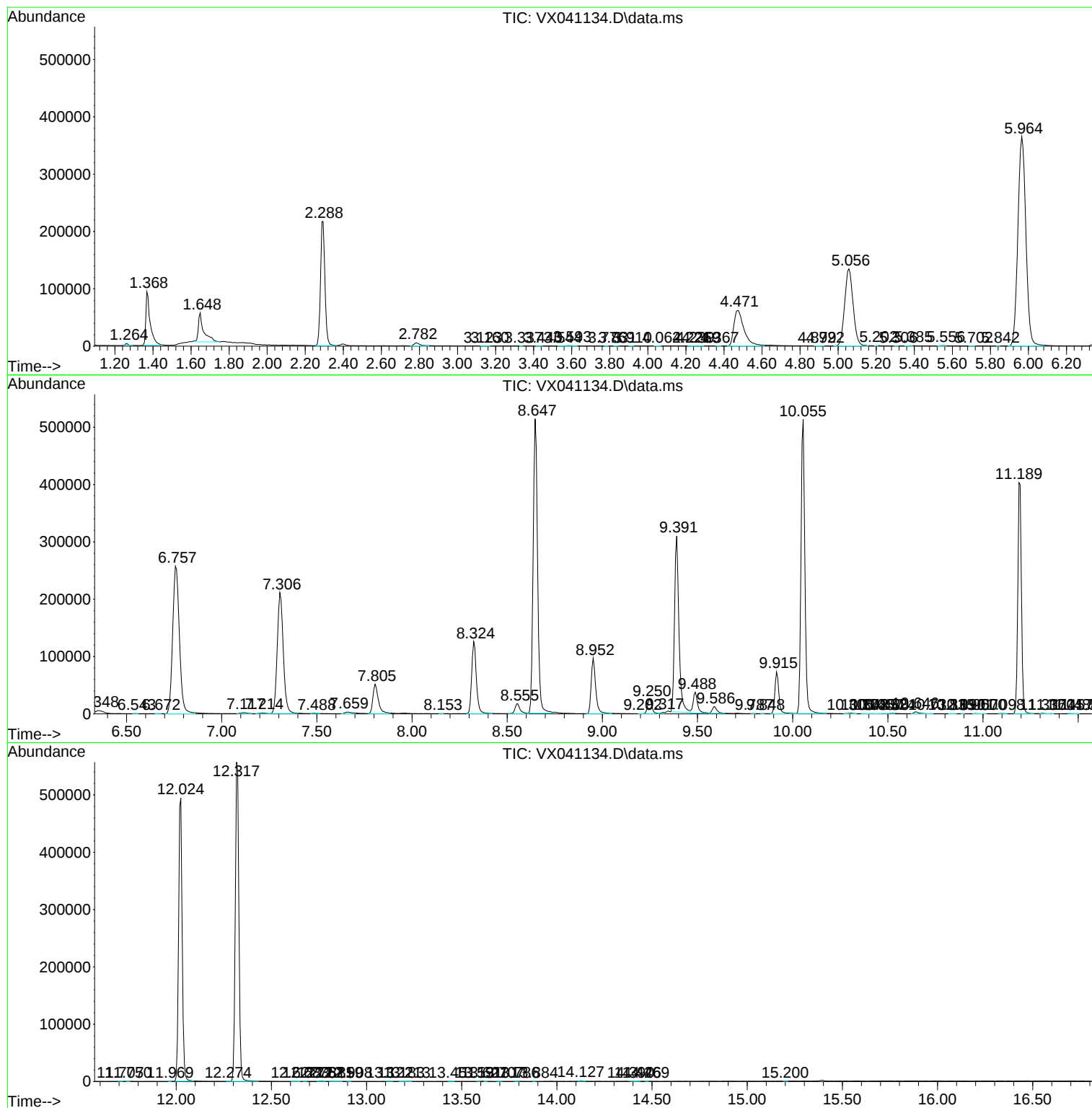
Sum of corrected areas: 8146778

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Instrument :
MSVOA_X
ClientSampleId :
E1CY1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
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E1CY1

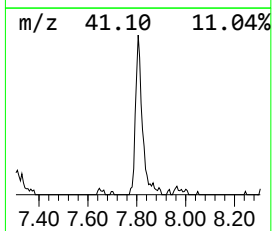
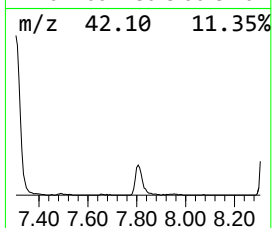
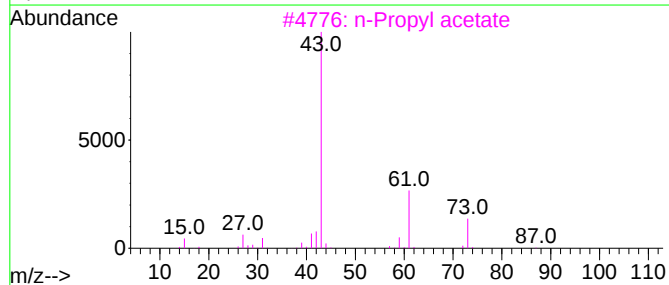
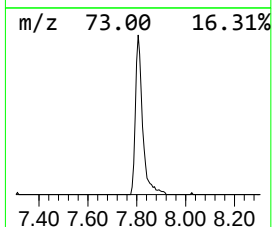
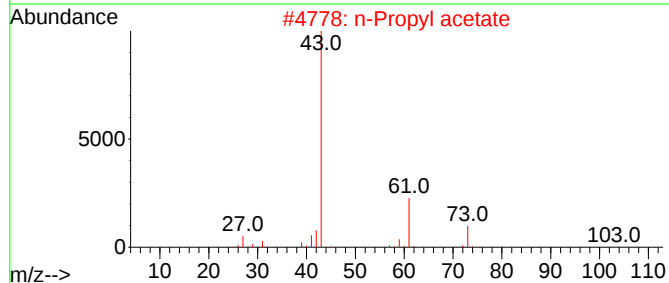
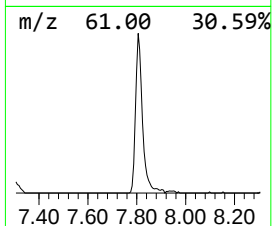
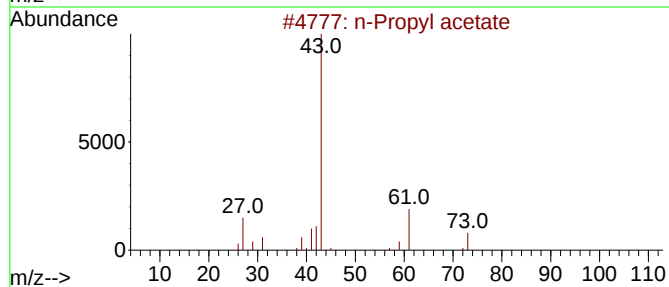
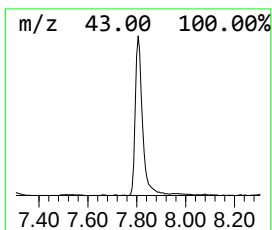
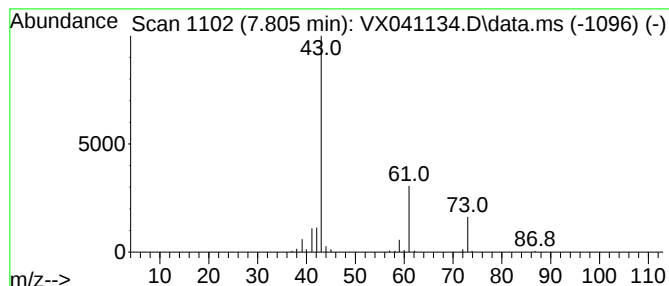
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.805	8.07 ug/L	101485	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	78
2	n-Propyl acetate			102	C5H10O2	000109-60-4	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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Instrument :
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ClientSampleId :
E1CY1

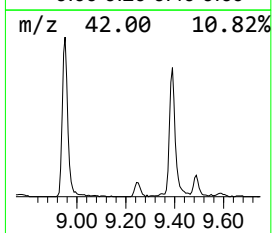
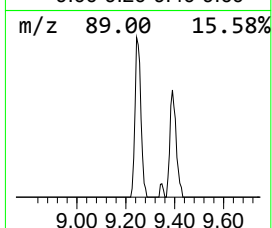
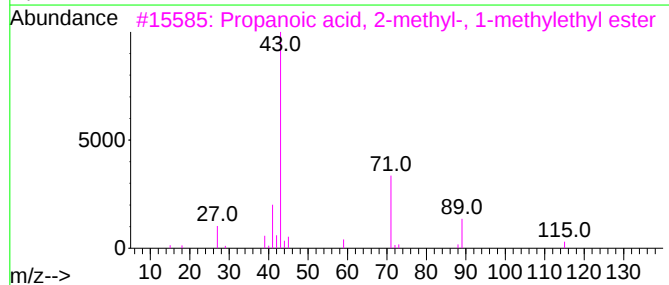
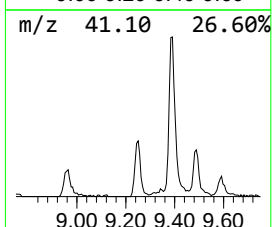
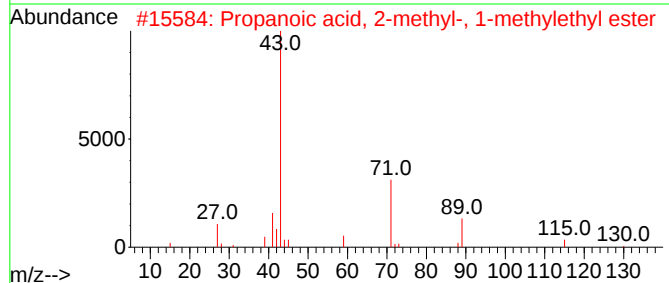
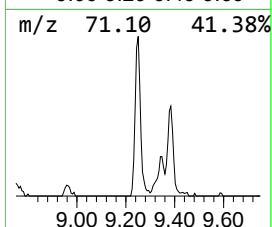
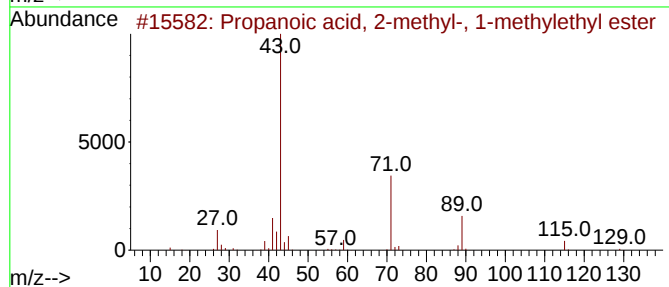
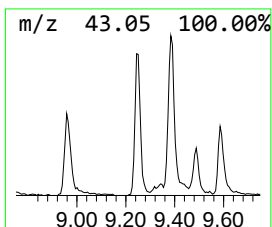
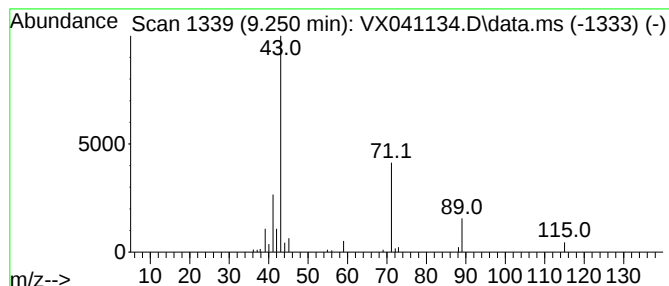
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.250	2.73 ug/L	39627	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



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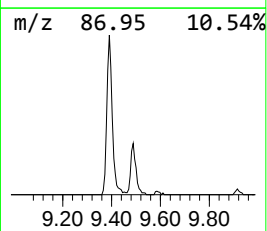
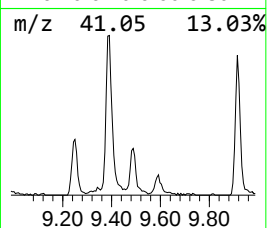
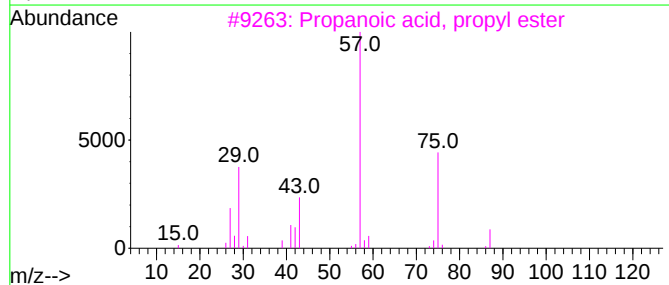
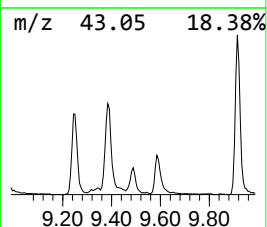
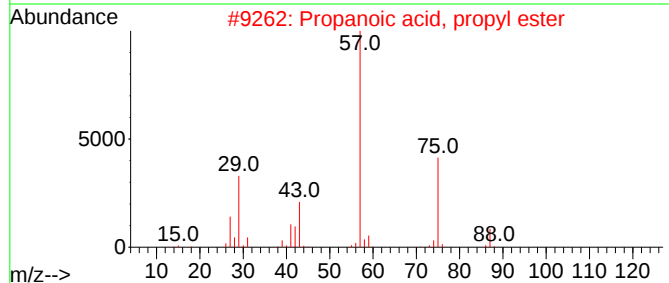
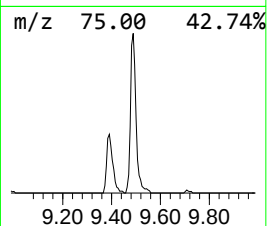
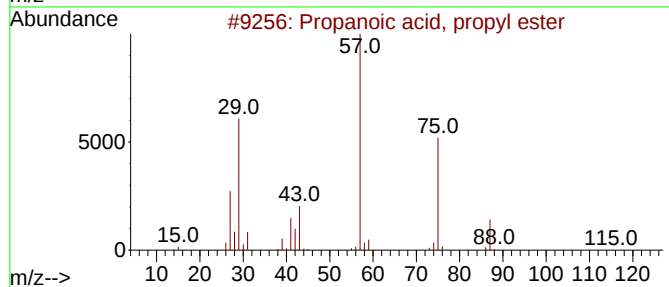
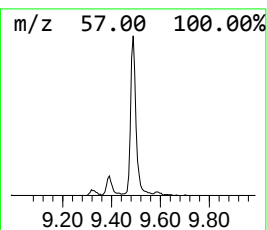
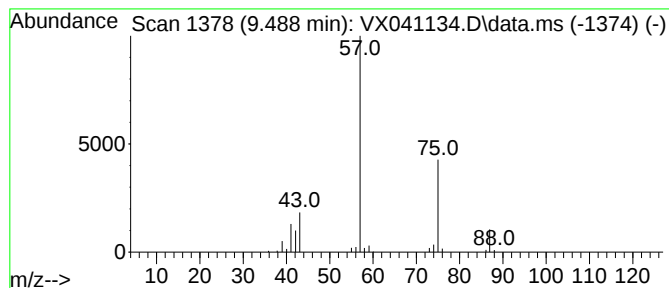
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041724WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	3.93 ug/L	57077	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041724\
Data File : VX041134.D
Acq On : 17 Apr 2024 18:48
Operator : JC/MD
Sample : P2039-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E1CY1

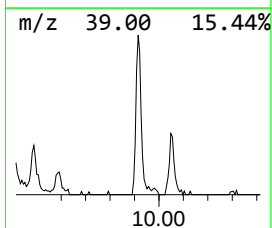
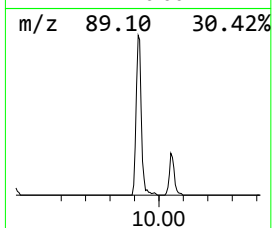
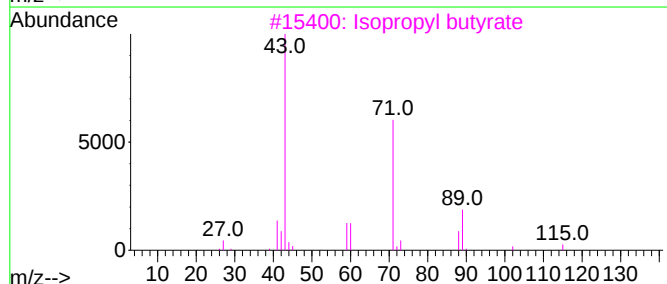
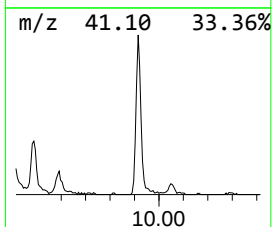
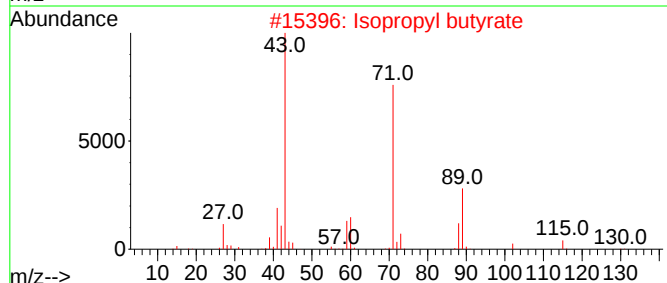
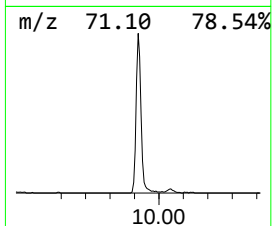
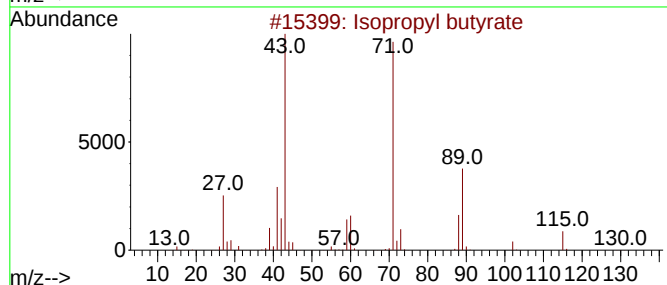
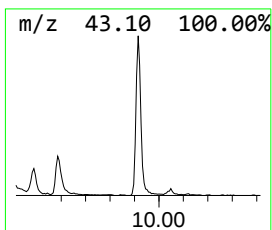
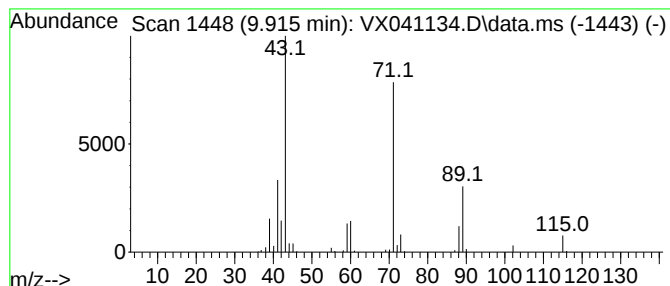
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	7.28 ug/L	105616	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041724\
Data File : VX041134.D
Acq On : 17 Apr 2024 18:48
Operator : JC/MD
Sample : P2039-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E1CY1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.805	8.1	ug/L	101485	1	6.757	629028	50.0
Propanoic acid,...	9.250	2.7	ug/L	39627	2	10.055	725494	50.0
Propanoic acid,...	9.488	3.9	ug/L	57077	2	10.055	725494	50.0
Isopropyl butyrate	9.915	7.3	ug/L	105616	2	10.055	725494	50.0